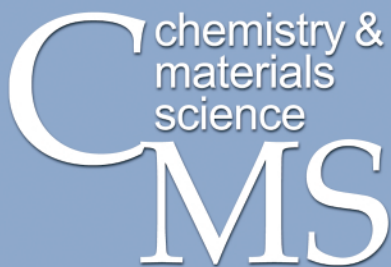


Chemistry and Materials Science Directorate News



April 2003
Volume 1, No. 2

Featured Articles:

***Molecular Modeling**

***Successful DRC Meeting**

***FSC Team at the World Series**



We are off to a running start this year...

We just completed our first Director's Review Committee (DRC) meeting in late-February. We highlighted scientific strengths and programmatic contributions in areas of Nonproliferation, Arms Control and International Security (NAI) as well as Homeland Security (HS). We also highlighted our very strong workforce. Please

(continued on page 2)

Providing scientific excellence and leadership that meets and anticipates the needs of the Laboratory's programs.

A corner on science...

Molecular modeling of aging processes

As everyone over 30 knows, aging is a part of life. We are using molecular simulation techniques to gain insight into fundamental aging processes of organic materials. Our calculations are focused around the issue of high explosive aging: "how old can an explosive get and still work reliably"? A plastic bonded explosive is a mixture of organic crystals of differing sizes (usually

between 1 and 100mm) held together with a polymeric "binder". Thus, in our aging studies we need to understand slow processes affecting packed powders and polymers.

While our studies are important for national security, they also raise interesting basic scientific questions. In our studies of packed powders, we have learned how to perform multi-scale simulations that seamlessly progress from length scales of 10^{-9} m to 10^{-4} m. We have learned that coarse-graining techniques must be carefully applied with an eye to maintaining fidelity to the essential processes of interest.

(continued on page 2)

The FSC Team was Awesome at the World Series

Our team fielded a win-win scenario...

Our focus was on the game, of course, and our goal was to win without any losers. Our Forensic Sciences Center (FSC) team joined other agencies such as the FBI, California National Guard Civil Support Team, and SWAT to ensure the safety of everyone—as transparently as possible. In the event of a terrorist attack and/or chemical warfare release, the FSC team is ready to respond with accuracy, providing a quick response so that other agencies can do their job effectively. The FSC's role is to use the solid-phase microextraction (SPME) and portable gas chromatograph-mass spectrometer (GC-MS) to analyze any unknown chemicals in the field—and "field" in this case is certainly appropriate.



The FSC team at Home Plate after the 7th inning (from left to right: Del Eckels, engineer, ME; Peter Nunes, chemist, FSC; Gregory Klunder, staff scientist, FSC).

Prior to the game the FSC team took background samples of the stadium using the SPME tools. These portable analysis capabilities provide an important advantage when dealing with substances that

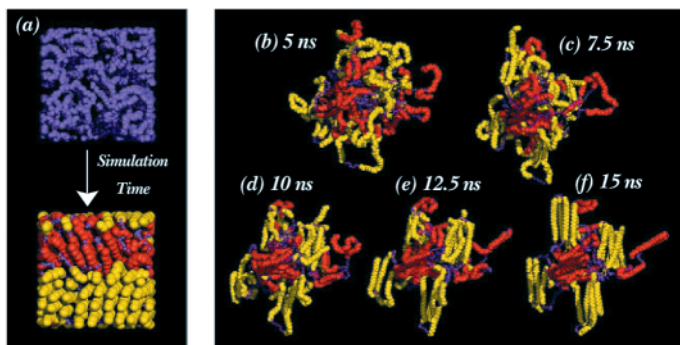
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"Molecular Modeling" *continued from page 1*

Our studies of polymers have been focused around the issues of crystallinity. Many polymers have a mixture of crystalline and amorphous regions. The mechanical properties of the polymer are strongly influenced by the size and shape of the crystalline regions. We have performed the first atomistic simulations of bulk polymer crystallization. These simulations require the use of

hundreds of processes for several months. The result is a unique understanding into the first events controlling polymer crystallization.

The authors, Richard Gee and Laurence Fried, support CMS' Chemistry & Chemical Engineering Division in the Energetic Materials Center which implements LLNL's energetic materials research and development program in support of Stockpile Stewardship. Published in: *J. Chem. Phys.* **118**(8), 3827 (2003).



The graphic shows initial and final configurations of a model poly(vinylidene fluoride) polymer (a). Time evolution of the pVDF crystal nucleation and growth process "loops" into and out of the crystal lamella and "amorphous" regions are colored purple. Only the carbon backbone atoms are shown for clarity. Chain segments colored red and yellow (space-filling representation) illustrate the polycrystalline nature of the ensemble.

"World Series" *continued from page 1*

may be unstable, perishable, or too toxic to bring back to the Laboratory. And, in the case of the World Series, allows the other teams (especially the baseball teams) to do their job with confidence. The center's approach to forensic analysis maximizes the information that can be obtained from sometimes small samples. Fortunately, nothing was found that would be suspect. But, even extremely small samples of explosives residue, dust particles, hair strands, blood stains, radioactive

isotopes, drugs, chemicals and clothing fibers can provide compelling evidence and will leave a chemical or biological signature that can be investigated.

The 2002 World Series was an important and high profile deployment for the FSC, and everything went extremely well. However, the San Francisco Giants' loss in game seven made for a somber trip back to the Bay Area for the FSC team. Oh well, maybe next year.

"Running Start" *continued from page 1*

see the section in this issue of our *Newsletter* that provides extensive information about the DRC and its presentations.

CMS is well positioned, and has anticipated the institutional need for science at the interface of chemistry, biology and materials science. We have been pro-active in formulation of the BioSecurity and Nanosciences Laboratory (BSNL) as a unique research and development initiative, and our long standing strong leadership in the Forensic Science Center continues to bear fruit. As the DRC pointed out, the science in the BSNL is world class, and the quality and enthusiasm of the workforce are second to none.

The DRC for CMS was impressed by our science and our workforce, both of which qualified as outstanding—the highest possible grade granted by a DRC. The grade for programmatic contributions will be assigned by the NAI/HS DRC based on our contributions as well as those from NAI and other organizations. Based on what we heard over two days of talks, posters and laboratory tours, the DRC members were impressed with our programmatic contributions. They also provided many useful comments. Over the next few weeks, we will be providing their comments to all of the presenters and participants in the review. Congratulations to everyone in the Directorate!

As many of you know, the Laboratory is currently in the process of developing a strategic plan for its science and technology (S&T) investments. Hal Graboske, the Deputy Director for S&T (acting), is leading the effort. The goal is to have a clear investment philosophy for the S&T portfolio of the Laboratory that leads to compelling science—enhancing our existing missions and enabling

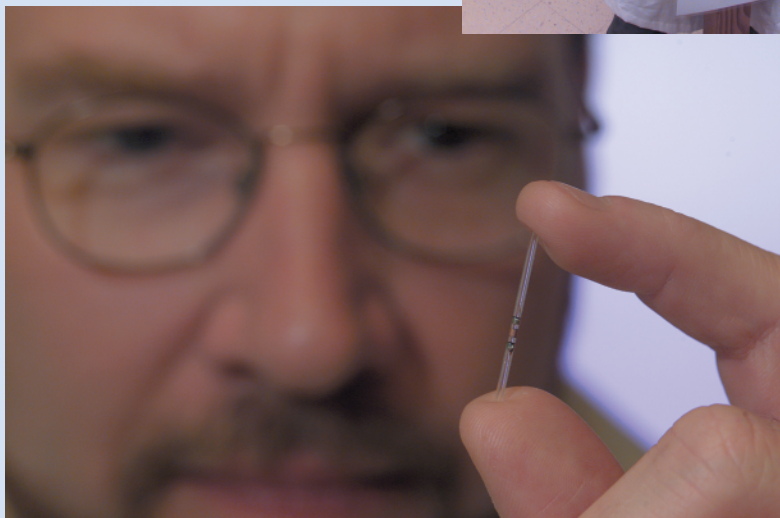
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"Running Start"
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What's new with our Facilities

We are pleased to announce the formation of a new center of excellence (CNSAMR-Center for National Security Applications of Magnetic Resonance), combining Nuclear Magnetic Resonance (NMR) expertise in materials characterization and structural biology. The center will join the NMR facilities in the Biological and Biosciences Research Program (BBRP) and CMS into a single facility in Building 151. The relocation will create a multidisciplinary, state-of-the-art facility dedicated to the cost effective and timely application of advanced NMR based methods to issues of national security. A suite of NMR instrumentation capable of meeting the broad scope of technological needs of various Laboratory programs has been assembled, including solid- and solution-state NMR capabilities as well as micro-imaging (MRI) facilities. The center will provide

LLNL programs with a unique resource for the elucidation of chemical, physical, structural, dynamic, and mechanical properties of a broad range of materials (biologic, organic, and inorganic).



future ones. One of my tasks will be to co-lead the development of plans for two of the six investment areas. As a team, Bruce Goodwin and I are developing plans for *Stockpile Science and Technology*. Another team effort will be working with Bert Weinstein to develop a plan that merges science and technology in biology, and the chemical and materials sciences. Many senior CMS scientists have been, and continue to be, involved in these two areas as well as in the development of plans of the other four S&T efforts, namely high energy density, nuclear and radiation, information systems, and energy and environment. The process is on a relatively fast pace, and we expect to present detailed plans to Director Mike Anastasio in early April. I will discuss the outcome of this process in our July *Newsletter*.

Again, many thanks to those of you who presented at the DRC, your material was well-received and certainly supports our scientific themes for the Directorate. The quality of all the presentations reflected extremely well on our drive for excellence in the chemical and materials sciences in support of our national security mission. It was clear from the review that we are delivering on our commitments to the Laboratory, and are very well positioned to capitalize on future opportunities through innovation in science and technology. Also, thanks to Jeff Kass and the Directorate's administrative staff for a great job of putting together and executing a flawless program. This is a tremendous start for the year, and a pattern of success that I look forward to in the future.

Cheers, Tomas



Success at our First DRC Meeting—Good Stuff!

It's a pleasure to report that the DRC committee had high praise for the Directorate's work and its dynamic team of scientists.

On February 25–27, 2003 the CMS Directorate held its first Director's Review Committee (DRC) meeting, the second meeting is scheduled for late May. The DRC is comprised of 15 distinguished scientists drawn from across the United States who provide an assessment of the quality of our scientific research, our support to the programs, and our management of the Directorate. The committee also provides advice to help us address our many challenges. Professor Tom Tombrello, Chairman of the Department of Physics at Cal Tech University, is chairman of the committee. This year the committee was substantially revised to reflect our broadened mission. The DRC focused on our increasing efforts in *science at the intersection of chemistry and biology*, and our strong support of NAI and Homeland Security.

Introductions and a Focus on the Directorate's Themes for the Future

Mike Anastasio, our LLNL Director, greeted the committee; Hal Graboske, Acting Deputy Director for Science and Technology, emphasized the importance of science and technology to support the Laboratory's long-range national security mission, and the impact the committee's review would have on LLNL's performance by the NNSA and the University of California; and Tomas Diaz de la Rubia highlighted the importance of integrating excellence in science and technology with that of operations, and defined the Directorate's strategy and its focus on four themes:

- Materials under extreme conditions;
- Chemical engineering and chemistry under extreme conditions;
- Science in support of national security at the intersection of chemistry, biology and materials; and
- Applied nuclear science for human health and national security.

Charles Westbrook provided an update of the impressive number of publications produced by our CMS staff since the last review. (Also see the related article in this issue: **We have a new CMS Database!**)

In Support of NAI, Homeland Security, and the Role of the BSNL

Wayne Shotts, Associate Director for NAI and Homeland Security, described LLNL's contribution to these very important national programs and emphasized the importance of CMS and the great job it is doing to accomplish these goals. César Pruneda discussed the comprehensive support CMS provides to all the programs. Bill Colston, Associate Program Leader for NAI's Bio Detection Chemical and Biological National Security Program, reiterated the threat the United States faces regarding bioterrorism and the need for the BioSecurity and Nanosciences Laboratory (BSNL). Jim De Yoreo presented an overview of the BSNL and its pivotal role in scientific research to protect the nation against biological threats and diseases. The BSNL presentations were as follows:

- Thomas Huser—summarized his research on nano- and bio-photonics to provide new directions for the development of single-molecule pathogen detection and increasing our understanding of protein-protein inter- and intra-molecular interactions.
- Chris Mundy—discussed ab initio modeling of the physical and chemical properties of aerosols. He demonstrated that harnessing LLNL's unique terascale computational capability enables realistic simulations of the fate and transport of biological agents and environmental pollutants and emphasized that this research concurrently provides an opportunity to answer fundamental questions in interfacial science.

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*“DRC Meeting”
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Poster Sessions Highlighting the BSNL

Ten posters were presented, followed by a tour of the BSNL conducted by Chris Hollars. During the tour, the participants discussed single molecule fluorescence.



- Julie Perkins—showed how we have developed and demonstrated an approach to synthesizing synthetic high-affinity ligands, designed to bind to target proteins with high affinity and specificity. This research has direct application to bio-warfare agent detection and delivery of radiation treatment to cancer cells.
- Roger Qiu—described the first molecular-scale picture of calcium-oxalate growth and modification by naturally occurring proteins and therapeutic agents. This work is laying the foundation for understanding the occurrence and treatment of kidney stone disease.
- Andrew Quong—described multi-length-scale modeling capability to understand and predict human-host response to pathogen exposure.
- Julio Camarero—described a possible route to direct interrogation of protein-protein interactions and elimination of macromolecular crystallization as the barrier to protein structure determination.
- Sonia Létant—described the first functionalized silicon membranes and demonstrated their use for the selective capture of simulated bio-organisms. This research opens the door on a new class of sensors able to collect and detect bio-organisms in the field and in real time.
- Aleksandr Noy—showed that the force needed to break solid-solid contacts in fluids is influenced by the structure of the solvent. These findings establish a new paradigm for understanding molecular adhesion in solutions as well as a quantitative method for its measurement and analysis.
- Charlene Schaldach—described a suite of advanced analytical tools to characterize biological agents and the processes by which they were made. By creating a biological signatures database we are building toward a National BioForensics Information System.
- Eric Gard—described the use of laser ionization and time-of-flight mass spectroscopy to detect/analyze the composition of bio-aerosols.
- Olga Bakajin—described a process for new nanotube-based device architectures, developed approaches for nanotube nanosensor platforms and explored the scientific basis for rational nanotube-based collector design.
- Lori Zeller—presented an analysis of complex biological mixtures for disease detection and prevention.

Challenges of our National Security Mission

David Eaglesham had an excellent strategic view describing the challenges and opportunities in the very dynamic Homeland Security mission, calling for the establishment of a ***national bio-warfare shield***. He emphasized that LLNL's greatest asset is its outstanding workforce. Dave's talk was followed by a series of interviews involving small groups of the CMS leadership team with the Review Committee. Other presentations were as follows:



- Bob Maxwell—discussed the LLNL Center for National Security Applications of Magnetic Resonance. (See the article in this *Newsletter* on the new facility.)
- Ian Hutcheon—described characterization of meteoritics with unique capabilities in mass spectrometry to date the oldest objects in the solar system.
- Dave Shoemaker—Classified talk on CAPS.
- Nathan Wimer—Classified talk on nuclear attribution.

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"DRC Meeting"
continued from page 5

An Emphasis on Counter-terrorism and Counter-proliferation

Harry Vantine, NAI R Program Leader, gave an overview of the Counter-terrorism and Incident Response Program and discussed Homeland Security needs for chemical radiation, nuclear and explosive threats. He emphasized the importance of CMS' support and that the CMS team was doing an excellent job. Specific presentations were:



- Judy Kammeraad—discussed nuclear detection and her work in gamma-ray imagers to improve the ability to find weak radiation sources amidst background radiation and legitimate radioactive objects.
- Glenn Fox—described the FSC's unique diagnostic and forensic capabilities for nuclear, chemical, and biological threats.
- Brad Hart—described research on new nanostructured materials for counter-proliferation and biological applications that have greater specificity over existing materials and greater integrity in harsh environments.
- Ian Hutcheon—discussed nuclear forensics and LLNL's work in support of world-wide efforts to prevent nuclear smuggling.

Poster Sessions on Nuclear Detection and Forensic Science



This session described CMS' work in nuclear detection and attribution as well as important work in the FSC. Glenn Fox conducted a tour of the FSC following the poster presentations:

- Howard Hall—new detector technologies for deployment, as well as systems tests at JFK airport in New York City.
- Tzu-Fang Wang—development of a new detector requiring very low power, with low cost, and high sensitivity.
- Jeff Haas—development and applications for explosives screening, detection, field deployment and monitoring.
- Peter Nunes—capability in support of various CONUS and OCONUS operations.
- Chad Talley—design of patterned nanostructured materials that may lead to array collectors and detector technology.
- Sharon Shields—highlighted an analytical interface for MALDI mass spectrometry, which allows LLNL scientists to determine basic chemical relationships between nanostructure materials and biological molecules for rapid separation and detection by mass spectrometry in array technology.
- Andy Vance—how the LLNL FSC is becoming the second U.S. designated laboratory certified by the Organization of Prohibition of Chemical Weapons (OPCW). To that end, the FSC has established an on-demand, state-of-the-art laboratory for synthesis of reference standards for chemical weapons and toxic industrial chemicals (TIC's) supporting detection (OPCW), environmental fate and intelligence programs.
- Gregory Klunder—FSC's unique capability in laser ablation mass spectroscopy for use in counter-proliferation forensic analysis.



Administrative Assistance

Several CMS administrators worked very hard to assure the high quality necessary for the review. They include Debbie Irish, Kristine Ramirez, Kim Hallock, Sally Hooper, Diana Bradbury, Trina Voelker, Katie Thomas, Lisa Palmer, Jana Marden, Patricia Martinez, Lisa Rose-McConville, Debbie Hackel, Kathy Silva, and Dabbie Schleich.



News about our Postdocs...

Julio Camarero and Olgica Bakajin are Lawrence Fellows working with our CMS staff. Both Julio and Olgica will be presenting results of their work in upcoming seminars as part of our BrownBag series.



Fitting into the goals of the Laboratory's future is a great feeling, and interacting with a multidisciplinary team of researchers to explore new frontiers in science is extremely motivating.

Julio was attracted to LLNL because of the opportunity to do great science and develop challenging new ideas at the interface between chemistry and biology. The promise of becoming integrated into a dynamic multidisciplinary team of scientists was also extremely attractive and a key factor in his decision to join the Laboratory. Julio's research interests focus

on one of the biggest challenges confronting us at the chem-bio interface: incorporating new synthetic amino acids into the universal genetic code used by all living organisms to biosynthesize proteins. Extending the chemical diversity of the universal genetic code will allow us to use the modern tools of organic chemistry to improve the stability, strength, and function of natural proteins, and to perhaps devise unnatural proteins with new functionality. His work at the Laboratory involves the development of new in vivo and in vitro methodologies for incorporating synthetic amino acids (fluorinated and perfluorinated amino acids, among others) into proteins to improve or modify their original function.



Having a group of young experts in various fields all working together on interdisciplinary problems is very exciting.

Olgica became interested in the Laboratory because of the dynamic team atmosphere at the BSNL. She really enjoys this unique opportunity to work with a diverse group of scientists. Olgica currently uses microfabrication and nanoscience to develop new

ways to concentrate, separate and detect bio and chem agents—critical components in counteracting bioterrorism and chemical warfare. She is also making new tools to study biomolecules which will help us understand mechanisms of the process of protein folding. This is important because various diseases such as mad cow, Alzheimer's and even some cancers occur when this process goes wrong.

Recent seminars at the Postdoc monthly BrownBag series include:

Feb 13: Dana Christensen, E&E, "Water Technology for the 21st Century"

Mar 20: Conversation with Tomas Diaz de la Rubia

Postdocs—coming or going?

Please welcome our new Postdocs:

ANCD: Julie Herberg

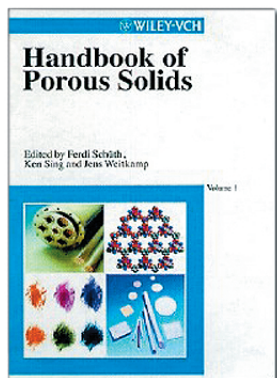
MSTD: Robert Meulenberg and Bryan Reed

Eduardo Bringa in MSTD will be leaving the Postdoc Program but will remain at LLNL, congratulations!

Notable PUBS

Aerogels: Making Light of Materials

Aerogels and other porous solids continue to be both scientifically interesting, and in the last two decades, very technologically important. LLNL's CMS scientists have been active participants and leaders in the development of porous materials, and particularly aerogels, for National Missions, and have lent their expertise in helping to solve problems for other agencies such as NASA (materials recovery from space), the auto industry (advanced catalysts), and the electronics industry (advanced inter-level dielectrics) to name just a few. Their leadership has recently been recognized in the **Handbook of Porous Solids**, edited by Ferdi Schüth, Ken Sing, and Jens Weitkamp, Wiley-VCH Verlag publishers, Weinheim, Germany (December, 2002).



Chapter 4 of this new reference book is titled "Oxidic Aerogels", and has been authored by CMS scientists, Ted Baumann, Alexander Gash, Glenn Fox, Joe Satcher, and Larry Hrubesh.

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Did you know?

We have a new CMS Database!

Every year there are multiple occasions when we are asked to provide data for review committees, DOE reports, and Directorate documentation. The intent of this database is to provide a convenient way of saving this information all year long and then assembling summaries very easily when needed. One recent request was for us to provide all the ongoing interactions with a particular university.

Thanks to Dannelle Tanner, who wrote a database management program using FileMaker Pro, we will be able to compile important information quickly to demonstrate our productivity. The database lists awards, books and book chapters, conference proceedings, papers, journal editorial boards we serve on, patents, refereed journal publications, and university collaborations. A goal is to also include whether information has been through the Review and Release process. To date,

2001 and 2002 information has been entered, although it's still a work in progress.

We will be asking each of you to review the database for accuracy and completeness in the coming months. The database is intended to be flexible enough to add any other classes of information that may be useful. Therefore, any suggestions and comments should be sent to Charlie Westbrook.

It's LDRD Season...

Spring is the season for LDRD...Labwide (LW) proposals are due March 21, Exploratory Research (ER) proposals are due May 9, and Strategic Initiatives (SI) proposals are due June 20. As a reminder, each of the major categories of LDRD is driven by its own Laboratory population and has a different focus and funding level. A good resource, especially for the LW projects: <http://ldrd.llnl.gov/ProposalSubmittal/LDRD.html>

"Notable PUBS" *continued from page 8*

These authors and their MIT collaborator Mildred Dresselhaus and her group have recently published four notable papers:

"*Synthesis and Characterization of Copper-Doped Carbon Aerogels*", *Langmuir* 2002,"**18**, pp7073-7076, <http://pubs3.acs.org/acs/journals/toc.page?incoden=langd5&indecade=0involume=18&inissue=18>

"*XPS Study of Copper-Doped Carbon Aerogels*", *Langmuir* 2002,"**18**, pp10100-10104, <http://pubs3.acs.org/acs/journalstoc.page?incoden=langd5&indecade=0involume=18&inissue=26>

"*Transport Properties of Copper-Doped Aerogels*", *Journal of Non-Crystalline Solids* **317** (2003) pp247-253, <http://www.sciencedirect.com>

"*The Growth of Carbon Nanostructures on Cobalt-Doped Carbon Aerogels*", *Journal of Non-Crystalline Solids* **318** (2003) pp223-232 <http://www.sciencedirect.com>

It's Pretty "Hot" in the Desert: Looking at our Nuclear Legacy

New Scientist, (8 February 2003, **177**, 2381, p.13) the weekly international science magazine, just completed an article "US Comes Clean on Nuclear Legacy" citing the manuscript authored by David

Smith and collaborators from LANL. Their paper will be appearing in the *Journal of Environmental Radioactivity* **67**(1), 35-51, 2003, "An inventory of long-lived radionuclides residual from underground nuclear testing at the Nevada test site, 1951-92", by D.K. Smith, D.L. Finnegan, and S.M. Bowen.

In this paper Dave and his co-investigators describe the source term at the Nevada Test Site that is a result of 828 underground tests between 1951 and 1992. The availability of these data affords an opportunity for the analysis of the radiologic term within the boundaries of local hydrogeologic units and provides insight to where radionuclides are sited relative to potential exposure pathways. This work is an important part of dealing responsibly with our nuclear legacy.

New Guidelines for the Recognition and Awards Program

New guidelines have been developed outlining our Recognition and Awards Program. These new guidelines provide consistency in awards distributions across the Directorate. The intent of this program is to promote and award excellence by recognizing

one-time achievements that have a notable impact on the Directorate or organization and/or contribute to the pursuit of excellence at LLNL. This differs from annual salary merit increases, which are in recognition of sustained performance.

Peer nominations are critical to the success of this program, and we encourage staff and management to nominate colleagues who they believe have had notable impacts through their accomplishments during the fiscal year. The nomination should reflect performance beyond that expected for such individuals and teams in the course of their assignment.

Highlights of the new guidelines include:

- The CMS Awards Program Committee. The committee consists of one scientific representative from each division and an administrative or technical representative from Operations. The charter of the committee is to review all award nominations for appropriateness and consistency across the Directorate. The committee will then make recommendations to the AD regarding the award type and monetary amount.
- Excellence in Publication Award. A new category that was added.

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*“New Guidelines”
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- A multi-tiered Directorate Awards Program:

—**Excellence Award**

Outstanding scientific accomplishment or discovery that receives national or international recognition; notable technical breakthrough that significantly enhances CMS’ ability to accomplish its mission and goals.

—**Exceptional Award**

Outstanding scientific, technical, or administrative innovation/invention/initiative that leads to important progress affecting many areas of research in CMS or toward the completion and/or success of an existing program.

—**Distinctive Award**

Significant scientific, technical, or administrative innovation that contributes to the completion and/or success of an existing program, or exemplary performance in response to an important organizational need.

New guidelines were distributed to all employees in March.

Check the website for information.

New Hires as of February 2003...Welcome!

ANCD	J. Herberg	PhD	Physics	University of Washington
ANCD	A. Winter	PhD	Metall. Eng.	Colorado School of Mines
ANCD	M. Chiarappa–Zucca	MS	Biology	University of Alabama
CChED	R. Upadhye	PhD	Chem. Eng.	University of California, Berkeley
MSTD	J. A. Caro	PhD	Physics	Swiss Federal Institute of Technology, Lausanne, Switzerland
MSTD	J. Hayes	MS	Mat. Eng.	Arizona State University, Tempe
MSTD	A. Malkin	PhD	Chemistry	Institute of Crystallography Soviet Academy of Sciences, Moscow USSR
MSTD	R. Meulenberg	PhD	Chemistry	University of California, Santa Barbara
MSTD	B. Reed	PhD	Applied Phys.	Cornell University



Chemistry and Materials Science Directorate News

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